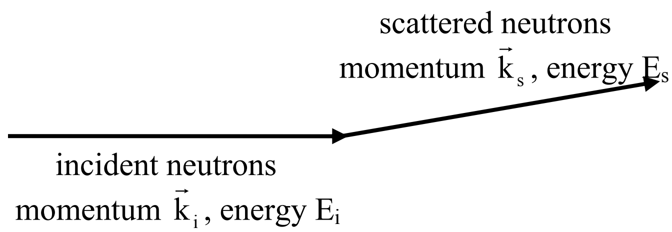
Chapter 8 - **ELASTIC AND QUASIELASTIC/ INELASTIC NEUTRON SCATTERING**

Structures are investigated using elastic scattering instruments whereas dynamics are probed using quasielastic/inelastic scattering instruments.

1. DEFINITIONS

Defining the momentum and energy for the incident neutron as ($\vec{k}_i$, E_i) and for the scattered neutron as ($\vec{k}_s$, E_s), the momentum transfer (scattering vector) is $\vec{Q} = \vec{k}_s - \vec{k}_i$ and the energy transfer is $E = E_s - E_i$ during the scattering event. Elastic scattering occurs when there is no energy transfer $E = 0$ (zero peak position and peak width). Inelastic scattering occurs when there is a transfer of both momentum and energy. Qasielastic scattering is a form of inelastic scattering where the energy transfer peak is located around $E = 0$ (zero peak position but with a finite peak width). In practice, the peak width is always limited by the instrumental energy resolution.



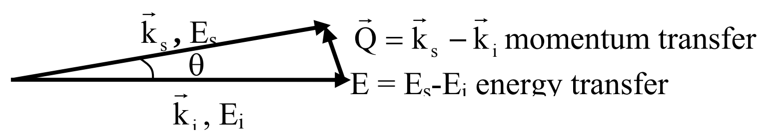


Figure 1: Schematic representation of the momentum and energy initial state ($\vec{k}_i$, E_i) and final state ($\vec{k}_s$, E_s).

2. SCATTERING SIZES AND ENERGY RANGES

The various elastic and quasielastic/inelastic neutron scattering instruments have specific window ranges in the (Q,E) space.

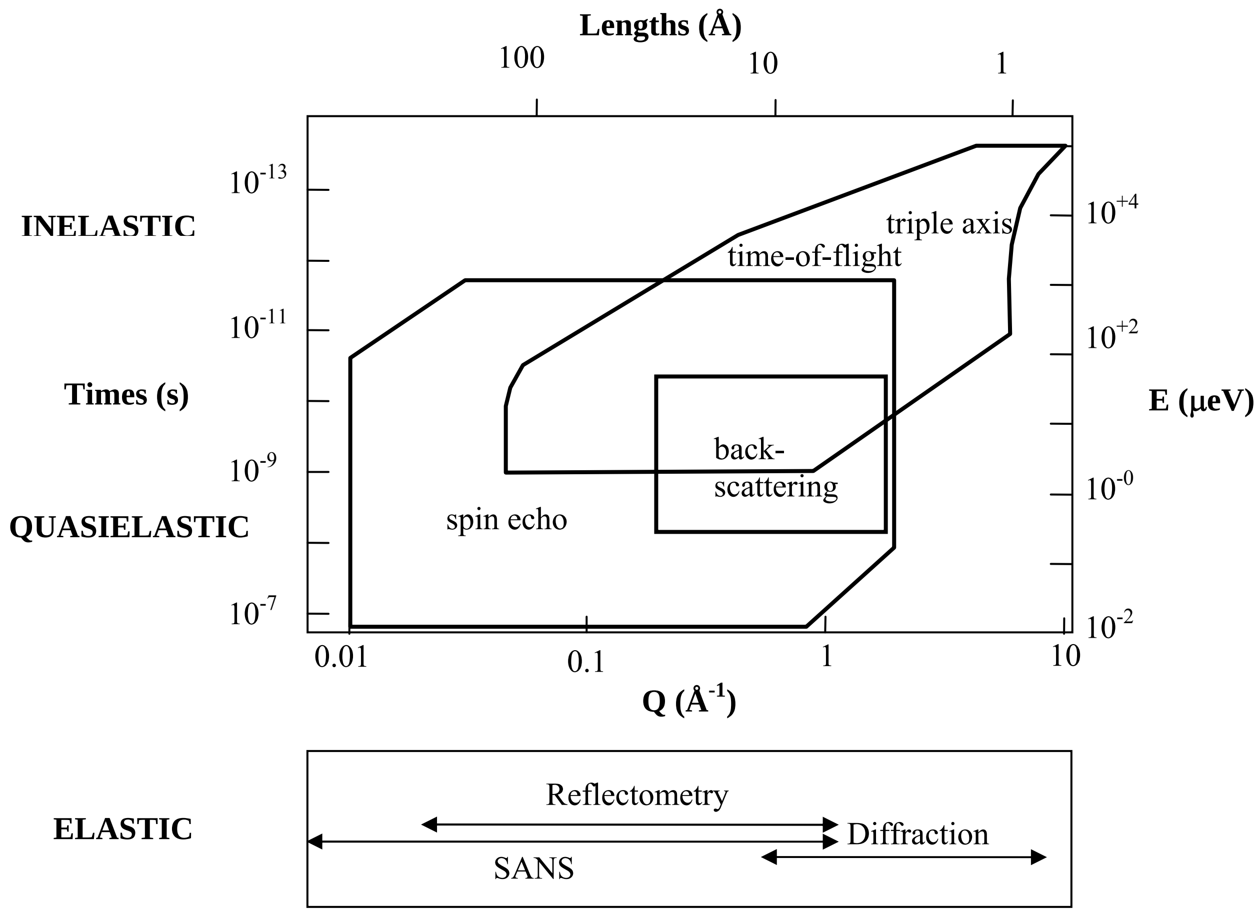


Figure 2: Schematic representation of the various elastic and quasielastic/inelastic neutron scattering instrument windows in (Q,E) space.

3. DIFFRACTION AND REFRACTION

Most neutron scattering methods operate in the "diffraction" mode. They involve single scattering and avoid multiple scattering events. Neutron reflectometry on the other hand operates in the "refraction" mode. It involves a large number of incremental scattering events that tend to steer the incident neutron beam until it is completely reflected. Describing reflection therefore involves a completely different theoretical basis than all other (single) scattering methods. The focus here will be on these methods that do not involve reflection. Within the first order perturbation theory, the so-called "master formula of neutron scattering" is derived next.

4. THE MASTER FORMULA OF NEUTRON SCATTERING

The single-scattering theory is based on the first Born approximation (the so-called Fermi Golden rule) describing s-wave scattering (Schiff, 1955; Bee, 1990). This corresponds to most forms of neutron scattering except for neutron reflectometry which requires higher order terms in the Born expansion. Defining an initial state for the neutron-nucleus system as |i> = $|\vec{k}_i\, n_i\rangle$ where $\vec{k}_i$ is the incident neutron momentum and n_i is the initial nuclear state and a scattered state as |s> = $|\vec{k}_s\, n_s\rangle$, the double differential neutron scattering cross section can expressed as:

$$\frac{d^2\sigma}{dEd\Omega} = \frac{k_s}{k_i} |< s | \left(\frac{m}{2\pi\hbar^2}\right) V(Q) | i >|^2 \; \delta(E - \mathcal{E}_s + \mathcal{E}_i) \tag{1}$$
$$= \left(\frac{m}{2\pi\hbar^2}\right)^2 \frac{k_s}{k_i} \sum_{n_i, n_s} P_{n_i} |< \vec{k}_s n_s | V(Q) | \vec{k}_i n_i >|^2 \delta(E - \mathcal{E}_s + \mathcal{E}_i).$$

Here m is the neutron mass, and P_{n_i} is the probability of finding a scattering nucleus in initial state $|n_i\rangle$. $\mathcal{E}_{n_i}$ and $\mathcal{E}_{n_s}$ are the energy states of the nucleus before and after scattering and V is the interaction potential. Note that due to the conservation of energy $\mathcal{E}_i - \mathcal{E}_s = E_i - E_s \sim E$ where E_i and E_s are the incident and scattering neutron energies and E is the transferred energy. Averaging over initial states and summing up over final states has also been performed.

Since neutron-nucleus interactions are short ranged, the following Fermi pseudo-potential is used.

$$V(r) = \left(\frac{2\pi\hbar^2}{m}\right) \sum_j^N b_j \delta(\vec{r} - \vec{r}_j). \tag{2}$$
$$V(Q) = \left(\frac{2\pi\hbar^2}{m}\right) \sum_j^N b_j \exp(-i\vec{Q}.\vec{r}_j)$$

Here b_j is the scattering length for nucleus j and N is the number of scattering nuclei in the sample. The following closure relation is introduced:

$$\int | \vec{r} > d\vec{r} < \vec{r} | = 1. \tag{3}$$

The <bra|ket> notation is used as follows:

$$< \vec{r} | \vec{k}_i >= \exp(i\vec{k}_i.\vec{r}) \tag{4}$$
$$< \vec{k}_s | \vec{r} >= \exp(-i\vec{k}_s.\vec{r})$$

The transition matrix element is calculated as:

$$< \vec{k}_s \,|\left(\frac{m}{2\pi\hbar^2}\right) V(Q)\,|\,\vec{k}_i >= \sum_j b_j < \vec{k}_s \,|\, \vec{r} > \int \delta(\vec{r}-\vec{r}_i)d\vec{r} < \vec{r}\,|\,\vec{k}_i > \qquad (5)$$

$$= \sum_j b_j \exp(-i\vec{Q}.\vec{r}_j)$$

Here $\vec{Q} = \vec{k}_s - \vec{k}_i$ and a property of the Dirac Delta function have been used. Moreover a special representation of the Delta function is used to express the following term as:

$$\delta(E - \mathcal{E}_s + \mathcal{E}_i) = \frac{2\pi}{\hbar} \int_{-\infty}^{+\infty} dt \exp\left(\frac{-i(E - \mathcal{E}_s + \mathcal{E}_i)t}{\hbar}\right). \qquad (6)$$

Finally the Heisenberg operator helps represent time dependence as follows:

$$\vec{r}_j(t) = \exp\left(\frac{-iHt}{\hbar}\right)\vec{r}_j(0)\exp\left(\frac{iHt}{\hbar}\right). \qquad (7)$$

Here H is the scattering system Hamiltonian.

$$H\,|\,n_i >= \mathcal{E}_i\,|\,n_i >,\ H\,|\,n_s >= \mathcal{E}_i\,|\,n_s >. \qquad (8)$$

Putting all terms together, the cross section is expressed as follows:

$$\frac{d^2\sigma}{dEd\Omega} = \frac{k_s}{k_i} \sum_{n_i,n_s} P_{n_i} \int_{-\infty}^{+\infty} dt \exp\left(\frac{iEt}{\hbar}\right) < n_s \,|\sum_{j,l} b_j b_l \exp\left(i\vec{Q}.\vec{r}_j(0)\right)\exp\left(-i\vec{Q}.\vec{r}_l(t)\right)|\, n_i >$$

$$= \frac{k_s}{k_i} S(Q,E). \qquad (9)$$

This is the most general neutron scattering cross section within the first order perturbation theory. The dynamic structure factor S(Q,E) has been defined in terms of the scattering density n(Q,t) as follows:

$$n(Q,t) = \sum_{j=1}^{N} b_j \exp\left(-i\vec{Q}.\vec{r}_j(t)\right) \qquad (10)$$

$$S(Q,E) = \frac{2\pi}{\hbar} \int_{-\infty}^{+\infty} dt \exp\left(\frac{-iEt}{\hbar}\right) < n(-Q,0)n(Q,t) >. \qquad (11)$$

The averaging notation $\sum_{n_i,n_s} P_{n_i} < n_s \,|\ldots|\, n_i >$ has also been simplified to <…>. The summations are over scattering nuclei. Note that at this level the scattering lengths are still included in n(Q,t) and in S(Q,E).

Note that the differential cross section $\frac{d\sigma(Q)}{d\Omega}$ used in elastic scattering is related to the double differential cross section $\frac{d^2\sigma(Q,E)}{dEd\Omega}$ used in quasielastic/inelastic scattering through an integral over energy transfers.

$$\frac{d\sigma(Q)}{d\Omega} = \int dE \frac{d^2\sigma(Q,E)}{dEd\Omega}. \tag{12}$$

There are many definitions for S(Q,E) in the literature.

5. THE VARIOUS STRUCTURE FACTORS

Many textbooks discuss the various structure factors (Bacon, 1962; Marshall-Lovesey, 1971). The Fourier transform of S(Q,E) is in the time domain.

$$S(Q,t) = \int_{-\infty}^{+\infty} dE \exp\left(\frac{iEt}{\hbar}\right) S(Q,E) \tag{13}$$

S(Q,t) is the time-dependent density-density correlation function also called time-dependent structure factor.

S(Q,E) is measured by most quasielastic/inelastic neutron scattering spectrometers such as the triple axis, the backscattering and the time-of-flight instruments. S(Q,t) is measured by the neutron spin echo instrument.

The initial value S(Q,t = 0) is the so-called static scattering factor S(Q). S(Q) is what diffractometers and SANS instruments measure. Note that S(Q) is also expressed as:

$$S(Q) = S(Q,t=0) = \int S(Q,E)dE. \tag{14}$$

Elastic scattering does not really mean with energy transfers E = 0 (zero peak and zero width); it rather means integrated over all energy transfers (summing up over all energy modes).

S(Q) is the density-density correlation function.

$$S(Q) = \langle n(-Q)n(Q) \rangle \tag{15}$$

Another form of the density-density correlation function S(Q) is related to the pair correlation function $g(\vec{r})$ through the space Fourier transform:

$$S(Q) = 1 + \overline{N} \int d\vec{r} \exp(-i\vec{Q}.\vec{r}) \left[g(\vec{r}) - 1 \right]. \qquad (16)$$

Here $\overline{N} = N/V$ is the particle number density. Note also that the scattering lengths have still not been separated out. These will be averaged for each scattering unit to form the contrast factor which will be multiplying S(Q).

REFERENCES

M. Bee, "Quasielastic Neutron Scattering", Adam Hilger (1990).

L.I. Schiff, "Quantum Mechanics", McGraw Hill (1955).

G.E. Bacon, "Neutron Diffraction", Oxford, Clarendon Press (1962).

W. Marshall and S.W. Lovesey, "Theory of Thermal Neutron Scattering", Clarendon Press, Oxford (1971).

QUESTIONS

1. What is the difference between quasielastic and inelastic scattering?
2. Define the terms in the following expression: $Q = \sqrt{k_i^2 + k_s^2 - 2k_i k_s \cos(\theta)}$.
3. What is "s-wave scattering"? What does it correspond to?
4. Can reflectometry data be described by the first Born approximation?
5. What is the Fermi pseudo-potential?
6. What is the differential cross section? How about the double differential cross section?
7. Write down the double differential cross section (the Master formula) for neutron scattering.

ANSWERS

1. Quasielastic scattering is characterized by energy transfer peaks centered at zero energy (with finite widths). Inelastic scattering is characterized by energy transfer peaks centered at finite energy (μev to meV).
2. k_i and k_s are the incident and scattered neutron momentums and θ is the scattering angle.
3. s-wave scattering corresponds to a zero angular orbital momentum (l = 0). It corresponds to single (not multiple) scattering.
4. Reflectometry involves refraction (not single diffraction). It cannot be described by first Born approximation. Higher order terms of the perturbation theory would have to be accounted for.

5. The Fermi pseudo-potential describes the short range neutron-nucleus interactions. It is formed of a series of Dirac Delta functions.

6. The differential cross section is $d\sigma/d\Omega$. The double differential cross section is $d^2\sigma/d\Omega dE$.

7. The double differential cross section is written as: $\frac{d^2\sigma}{dEd\Omega} = \frac{k_s}{k_i} S(Q,E)$. Here k_s and k_i are the scattering and incident neutron momentums and $S(Q,E)$ is the dynamic structure factor.